



CHEM 3P20
Library Seminar
Fall 2024

Ian Gordon



Ian Gordon, Teaching & Learning Librarian



Brock University Library

Library Seminar Agenda

- CHEM Library Research Guide
- Databases – lots of them!
- Citation management
- Where, how and when to get help

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<https://researchguides.library.brocku.ca/CHEM>

Chemistry

Chemistry retrofit guide by Ian

- WELCOME
- ARTICLES
- BOOKS
- CHEMICALS / DRUGS
- GREY LITERATURE
- DATA
- BORROW FROM OTHER LIBRARIES
- ADDITIONAL COURSE GUIDES

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Chemistry

What is this guide for?

This guide for chemistry has been designed as a general program guide and is curated by [Brock librarians](#). It features links to most often used resources such as databases for books, peer-reviewed journal articles, theses, dissertations, open educational resources (OERs), patents, standards, and more. Use the tabs on the left to navigate through the web page.

The [ACS Guide to Scholarly Communication](#) is an ACS publication that is constantly updated and provides access to the [ACS Quick Style Guide](#) that includes excellent information on writing, scholarship and style.

[CHEM 3P20 Library Seminar Fall 2024 ppt slides](#) (PDF)



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Articles

Journal articles are scholarly works that go through a quality control process called **peer-review** before they are published.

Several databases provide access to regional, national and international **news** articles.

A select list of **databases** that include scholarly articles are listed below.

The **ACS Guide to Scholarly Communication** is an ACS publication that is constantly updated and provides access to the **ACS Quick Style Guide** that includes excellent information on writing, scholar

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 - Includes Beilstein (to 1959, Supplement IV); Gmelin (to 1975); and selected organic chemistry patents (1869-1980) with English-language chemical patents (US, WO, EP, 1976+) from selected primary IPC classes.
 - For full usability set up an individual account for access on and off campus. Java and JRE plugins may be required.
 - **Permitted Uses**

Library Seminar Agenda

- CHEM Library Research Guide
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syntheses of morphine

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[\[PDF\] The **synthesis** of morphine](#)

M Gates, G Tschudi - Journal of the American Chemical Society, 1956 - ACS Publications

... have originated with Sertürner's¹ isolation of **morphine** from opium and his recognition of its ... for **morphine** (I). In this paper³ we describe the completion of the first **synthesis** of **morphine** ...

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[Synthesis of morphine alkaloids and derivatives](#)

U Rinner, T Hudlicky - Alkaloid **synthesis**, 2012 - Springer

... Since our update on **morphine synthesis** was published 5 years ... in the total **synthesis** of **morphine** alkaloids is depicted in ... a formal total **synthesis** of **morphine** as Rice demonstrated its ...

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[The quest for a practical **synthesis** of morphine alkaloids and their derivatives by chemoenzymatic methods](#)

JW Reed, T Hudlicky - Accounts of chemical research, 2015 - ACS Publications

... in chemoenzymatic **synthesis** that ... **synthesis**, including the various approaches to **morphine**, would have materialized. Here we trace the evolution of our approaches to **morphine** ...

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[Morphine synthesis and biosynthesis-an update](#)

BH Novak, T Hudlicky, JW Reed... - Current Organic ..., 2000 - ingentaconnect.com

... Abstract: This review covers recent developments in the area of **morphine synthesis** and ... advancements in biosynthesis of **morphine** alkaloids. Total **syntheses** published since 1996 ...

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[Formal **synthesis** of \(±\)-morphine.](#)

J Li, GL Liu, XH Zhao, JY Du, H Qu... - Chemistry-An Asian ..., 2013 - search.ebscohost.com

... the **synthesis** of the unique pentacyclic ring system with five contiguous stereocenters constitutes one of the most fascinating topics in the chemistry of **morphine** ... **synthesis** of **morphine**. ...

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Research Topic:

I want to find scholarly articles that focus on synthetic approaches to morphine, detailing specific experimental methods, catalysts, or novel pathways used in its synthesis.



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^ Detailed summary

A plethora of recent studies have centered on various synthetic approaches to morphine, utilizing novel pathways and catalysts to achieve efficiency and stereochemical control [1, 2, 3, 4].

Key Insights on Morphine Synthesis:

• Novel Pathways and Strategies:

- Recent syntheses have employed innovative techniques such as oxidative phenolic coupling and
- Biomimetic and chemoenzymatic methods have been explored, providing alternative strategies th

• Catalysts and Reagents:

- Asymmetric hydrogenations with organometallic catalysts have been pivotal, with advances in ca
- Enzymatic strategies and chemoenzymatic approaches, involving genetically engineered enzyme

• Efficiency and Stereoselectivity:

- Efficient total syntheses have been achieved with reduced steps and improved overall yields, lew
- Innovations in stereoselective transformations, such as sequential Claisen rearrangements, have

These findings highlight ongoing advancements in the field, focusing on optimizing reaction conditions a

∨ Categories of papers

∨ Timeline and citation network

∨ Discovery progress: ~52.2% complete (~20-27 papers found)

References

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Show only: ☐ Last 5 years ☐ Last 2 years ☐ > 1 citation per year ☐ > 5 citations per year

Topic Match	Cit./Year	Year	Paper
99.5%	3.9	2014	[1] Gram-scale enantioselective formal synthesis of morphine through an ortho-para oxidative phenolic coupling strategy. M. Tissot, ..., and M. Gaunt Angewandte Chemie 2014 - 38 citations - Show abstract - Cite
99.4%	3.0	2010	[2] Total synthesis of (-)-morphine. H. Koizumi, ..., and T. Fukuyama Chemistry, an Asian journal 2010 - 42 citations - Show abstract - Cite - PDF
99.3%	6.0	2002	[3] Synthesis of (-)-morphine. D. Taber, ..., and A. Rheingold Journal of the American Chemical Society 2002 - 132 citations - Show abstract - Cite
99.2%	2.8	2013	[4] Synthesis of (-)-morphine: application of sequential Claisen/Claisen rearrangement of an allylic vicinal diol. M. Ichiki, ..., and N. Chida Chemistry 2013 - 33 citations - Show abstract - Cite
99.1%	3.6	2017	[5] Total Synthesis of (-)-Morphine. Hirotatsu Umihara, ..., and T. Fukuyama Chemistry 2017 - 26 citations - Show abstract - Cite - PDF
99.1%	0.5	2006	[6] Syntheses of Morphine and Codeine (1992 - 2002): Templates for Exploration of Synthetic Tools L. Mascavage, ..., and D. R. Dalton Current Organic Synthesis 2006 - 9 citations - Show abstract - Cite - PDF
99.0%	0.3	2008	[7] A Practical Asymmetric Synthesis of the ACNO Fragment of Morphine Alkaloids L. Hsin, ..., and Hui-Ling Liou Synlett 2008 - 5 citations - Show abstract - Cite
98.9%	0.4	2006	[8] Chemoenzymatic Synthesis of Complex Natural and Unnatural Products: Morphine, Pancratistatin and Their Analogues T. Hudlický ChemInform 2006 - 7 citations - Show abstract - Cite
98.9%	7.0	2015	[9] The quest for a practical synthesis of morphine alkaloids and their derivatives by chemoenzymatic methods. J. W. Reed and T. Hudlický Accounts of chemical research 2015 - 67 citations - Show abstract - Cite

<https://chatgpt.com/>

top syntheses for morphine?

Morphine, an opiate used primarily for pain relief, is synthesized through various methods, but it's important to remember that handling and synthesizing controlled substances like morphine should be done only by qualified professionals in regulated environments due to legal and safety concerns.

Here are a few well-known synthetic approaches to morphine:

1. **Thebain-Based Synthesis:** The most common synthetic route starts from thebaine, a compound found in opium. The synthesis involves a series of chemical transformations, including:
 - **Hydrolysis** of thebaine to obtain oripavine.
 - **Reduction and rearrangement** to produce morphine.
2. **Total Synthesis from Simple Precursors:** This approach aims to construct morphine starting from simpler chemical entities. One notable method involves:
 - The use of intermediates like 3,6-dioxopiperidine and complex reactions to build the morphine structure from scratch.
3. **Semi-Synthesis from Codeine:** Codeine, another opiate present in opium, can be chemically modified to produce morphine:
 - **O-demethylation** of codeine can yield morphine through a series of reactions.
4. **Total Synthesis from Simple Chemicals:** This method involves building the morphine molecule entirely from simpler starting materials. A classic example is the synthesis developed by Robert Woodward and his team, which was one of the earliest total syntheses of morphine.
5. **Total Synthesis from Benzyloquinoline:** This involves using benzyloquinoline as a starting material and applying a series of chemical transformations to produce morphine.

These methods are typically complex and require a high level of expertise in organic chemistry. If you're interested in the detailed procedures, consulting scientific literature and chemical synthesis textbooks would be the best approach. Always ensure to follow legal regulations and safety guidelines when dealing with substances like morphine.



https://en.wikipedia.org/wiki/Total_synthesis_of_morphine_and_related_alkaloids

Total synthesis of morphine and related alkaloids

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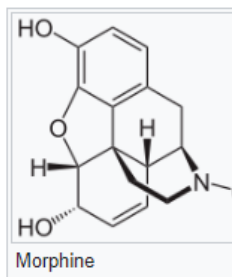
From Wikipedia, the free encyclopedia

Synthesis of morphine-like alkaloids in chemistry describes the **total synthesis** of the natural **morphinan** class of alkaloids that includes **codeine**, **morphine**, **oripavine**, and **thebaine** and the closely related **semisynthetic** analogs **methorphan**, **buprenorphine**, **hydromorphone**, **hydrocodone**, **isocodeine**, **naltrexone**, **nalbuphine**, **oxymorphone**, **oxycodone**, and **naloxone**.^{[1][2]}

The structure of morphine is not particularly complex, however the electrostatic polarization of adjacent bonded atoms does not alternate uniformly throughout the structure. This "dissonant connectivity" makes bond formation more difficult and therefore significantly complicates any synthetic strategy that is applied to this family of molecules.^[2]

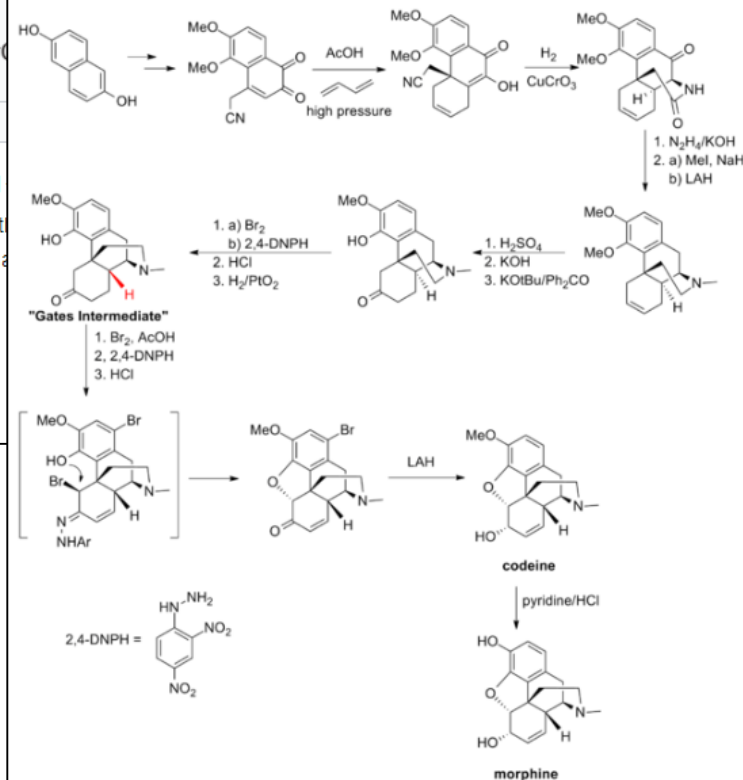
The first morphine total synthesis, devised by **Marshall D. Gates, Jr.** in 1952 remains a widely used example of total synthesis.^[3] synthesis took a total of 31 steps and proceeded in 0.06% overall yield. The **hydrocodone** synthesis of Kenner C. Rice is one of the most efficient and proceeds in 30% overall yield in 14 steps.^[4] At 9 steps, the Barriault route is the shortest to date, but contains a number of low-yielding steps and is racemic.^[5]

Several other syntheses were reported, notably by the research groups of **Evans**,^[6] **Fuchs**,^[7] **Parker**,^[8] **Overman**,^[9] **Mulzer-Trauner**,^[10] **White**,^[11] **Taber**,^[12] **Trost**,^[13] **Fukuyama**,^[14] **Guillou**,^[15] **Stork**,^[16] **Magnus**,^[17] **Smith**,^[18] and **Barriault**.^[5]



Gates synthesis [edit]

Gates' total synthesis of morphine^[3] provided a proof of the structure of morphine proposed by **Robinson** in 1925.^[19] morphine features one of the first examples of the **Diels-Alder reaction** in the context of total synthesis.^[3]



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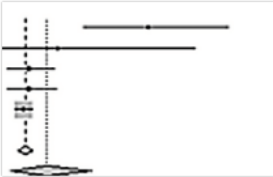
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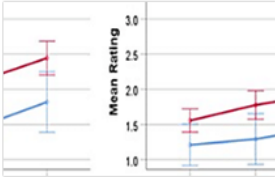
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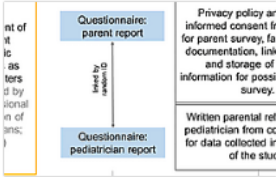
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Recruitment and study procedure.

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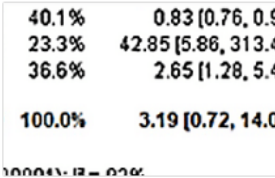
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Pooled prevalence of concentration difficulties in long COVID among childre...

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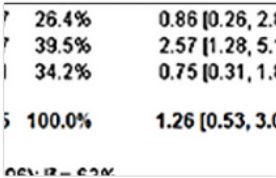
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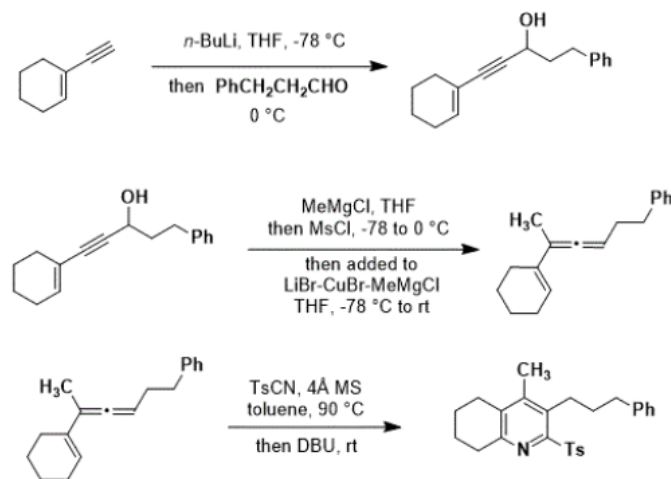
Preparation of Highly-Substituted Pyridines via Diels-Alder Reactions of Vinylallenes and Tosyl Cyanide

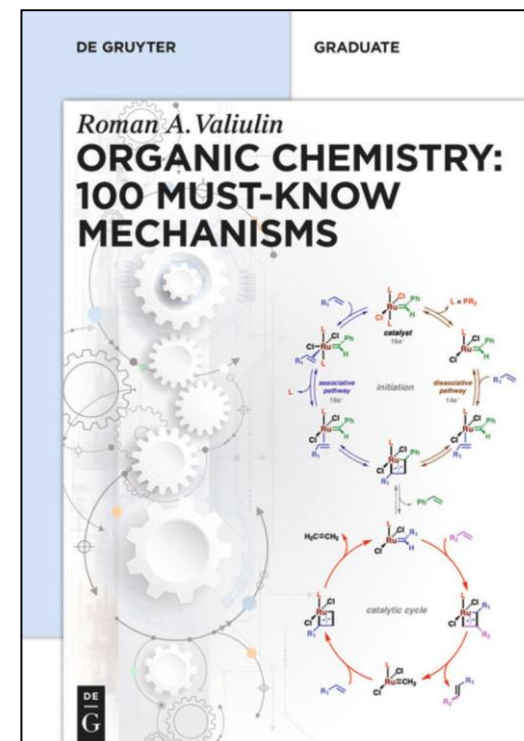
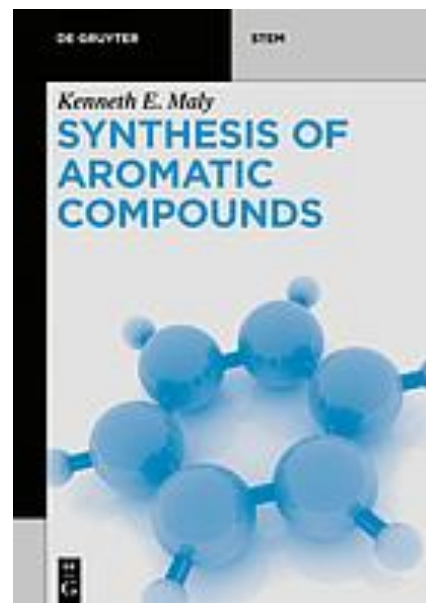
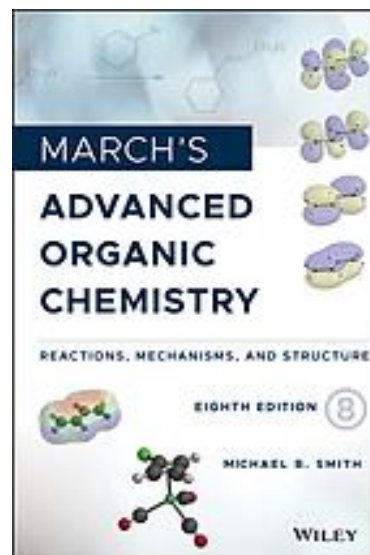
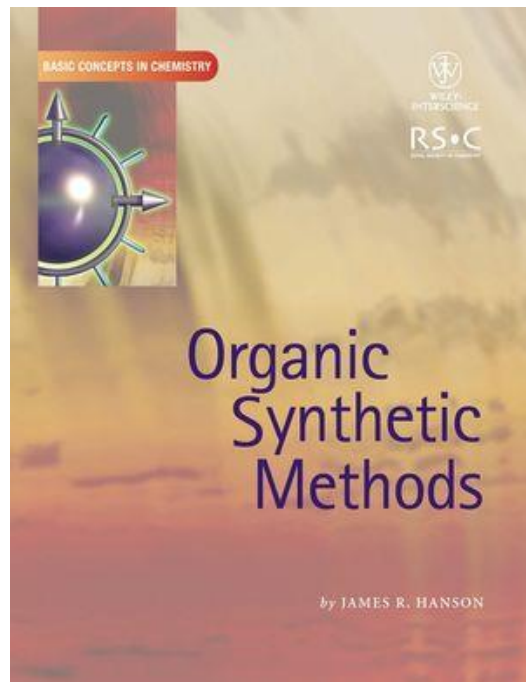
Nathan H. Faialaga, Christian Gomez, Samuel G. Bartko, Philipp Natho, and Rick L. Danheiser

Org. Synth. **2023**, *100*, 4

DOI: 10.15227/orgsyn.100.0004

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Definitions are scholarly dictionaries, encyclopedias and handbooks that help define terms and provide additional context.

Dictionary of Chemistry (2020) **Biochemistry and Molecular Biology** (2006) **Biomedicine** (2010)

Taber's Cyclopedic Medical Dictionary (2021)

Compendium of Chemical Terminology (current, IUPAC)

CRC Handbook of Chemistry & Physics (2014/2015)

Periodic Table Gallery (ACS)

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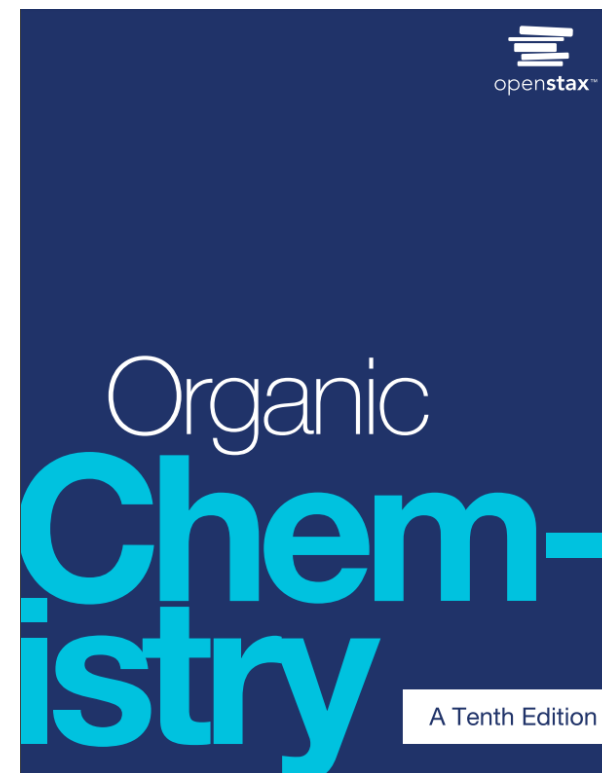
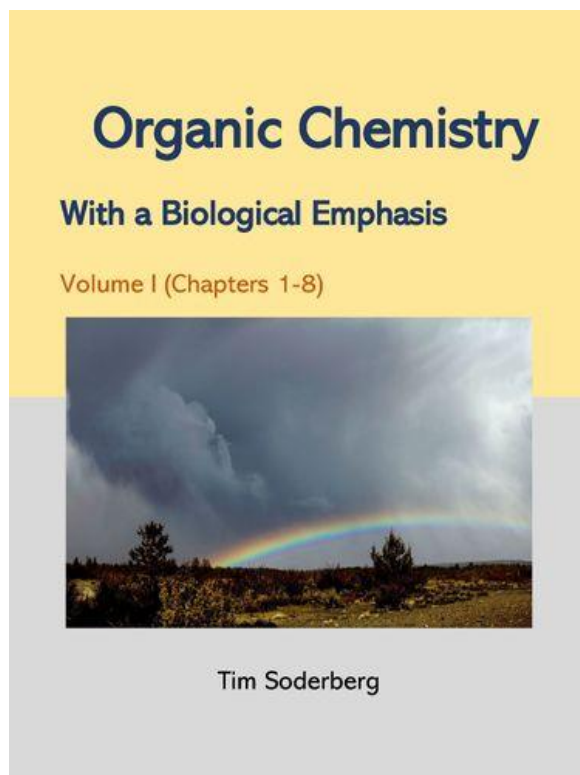
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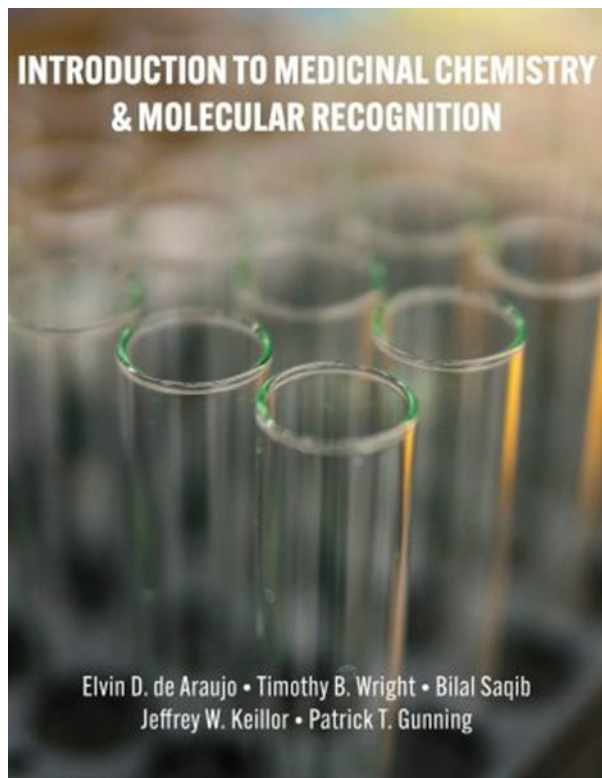
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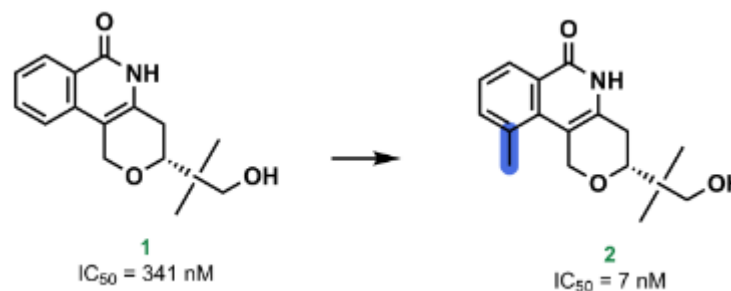
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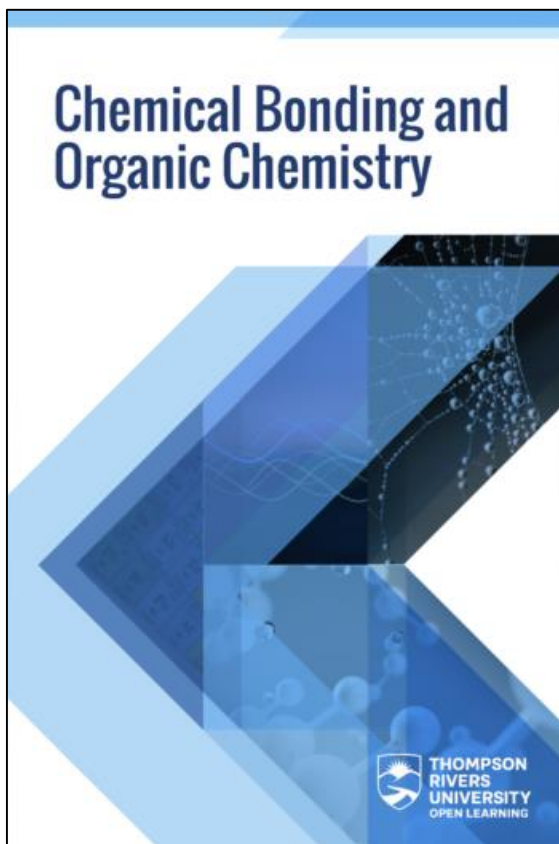


3.3 Binding is Determined by Drug : Target Interactions

Ultimately, the capacity of a drug to engage with a target is determined by the thermodynamic binding energy. In a reversible reaction, the target enzyme (E) will bind an inhibitor (I) to give the complex $E \cdot I$, where the equilibrium is governed by the constant K_d (or K_i in the presence of substrate). One of the main goals of medicinal chemistry and a significant portion of hit-to-lead investigations is to design molecules that will improve (decrease) the K_d . Understanding how to improve K_d , requires an understanding of the types of interactions that can occur between a target and its inhibitors. There are generally three types of binding interactions, i) electrostatic, ii) hydrogen bonding, and iii) “hydrophobic” interactions.



<https://openintrochemistry.pressbooks.tru.ca/>

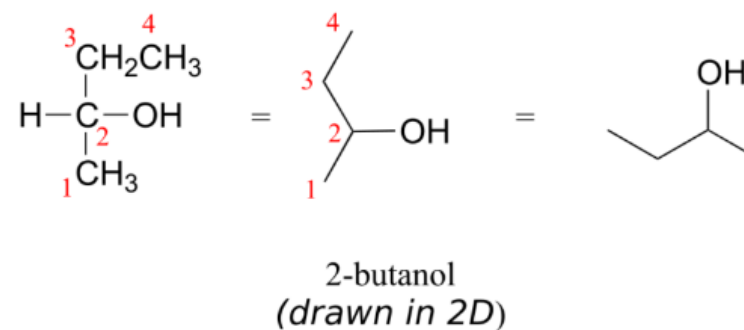


8.3 Stereochemistry of Organic Compounds and Pharmaceuticals

Chirality and Stereoisomers

We turn now to the concept of chirality that formed the basis of the story about Louis Pasteur in the beginning of this chapter. Recall that the term **chiral**, from the Greek work for “hand,” refers to anything which cannot be superimposed on its own mirror image. Your hands, of course, are chiral—you cannot superimpose your left hand on your right, and you cannot fit your left hand into a right-handed glove (which is also a chiral object). Chiral objects do not have a mirror plane. You cannot place your hand in such a way that one side is the mirror image of the other side. Chiral objects do not

Consider 2-butanol, drawn in two dimensions below.



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Syntheses of Morphine

by M Maier · 1995 · Cited by 9 — Since drugs have been known, they have been contested in society. This is quite understandable in the light of the misery and the crime.

People also ask

What is a synthetic version of morphine?



Can morphine be Synthesised?



What is a synthetic drug like morphine?



What is an opioid drug that is synthesized from morphine called?



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Syntheses in the Direction of Morphine. II.1 Some ...

by MD Soffer · 1950 · Cited by 37 — bined, and the early literature is in many cases incomplete and confused. (8) Cornforth, Cornforth and Robinson, J. Chem. Soc., 689. (1942).



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544. Syntheses in the Morphine Series. Part V.* Model

by D Elad · 1953 · Cited by 3 — IN Part IV * the synthesis of a tetracyclic compound (Ia) was described. This substance bears an oxygen function at C(5) which can be used as a key to...

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chemical predictive retrosynthesis database?

Alternate Databases

Open Reaction Database

<https://docs.open-reaction-database.org/>

PubChem

<https://pubchem.ncbi.nlm.nih.gov/>

KEGG Reaction Database

<https://www.genome.jp/kegg/reaction/>

Organic Chemistry portal

<https://www.organic-chemistry.org/>

ChemSpider

<https://www.chemspider.com/>

Chemicalize

<https://chemicalize.com/>

ChEMBL

<https://www.ebi.ac.uk/chembl/>

Predictive Restrosynthesis Databases

<https://www-library.ch.cam.ac.uk/list-useful-databases>

<https://askcos.mit.edu/>

Explore ASKCOS

Enter a molecule or reaction SMILES to explore available tasks



Type here or draw structure...



DRAW



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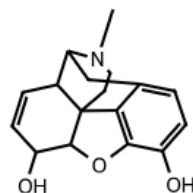
OC1C=CC2C34C1Oc1c4c(CC2N(CC3)C)ccc1O



DRAW



CANONICALIZE



SCScore

▶ EVALUATE

Interactive Path Planner

▶ PERFORM ONE-STEP

Tree Builder

▶ BUILD TREE ▼

Predict Forward Synthesis

▶ RUN TASK

Predict Impurities

▶ RUN TASK

Predict Aromatic Site Selectivity

▶ RUN TASK

Solvent Screen

▶ RUN TASK

Buyables

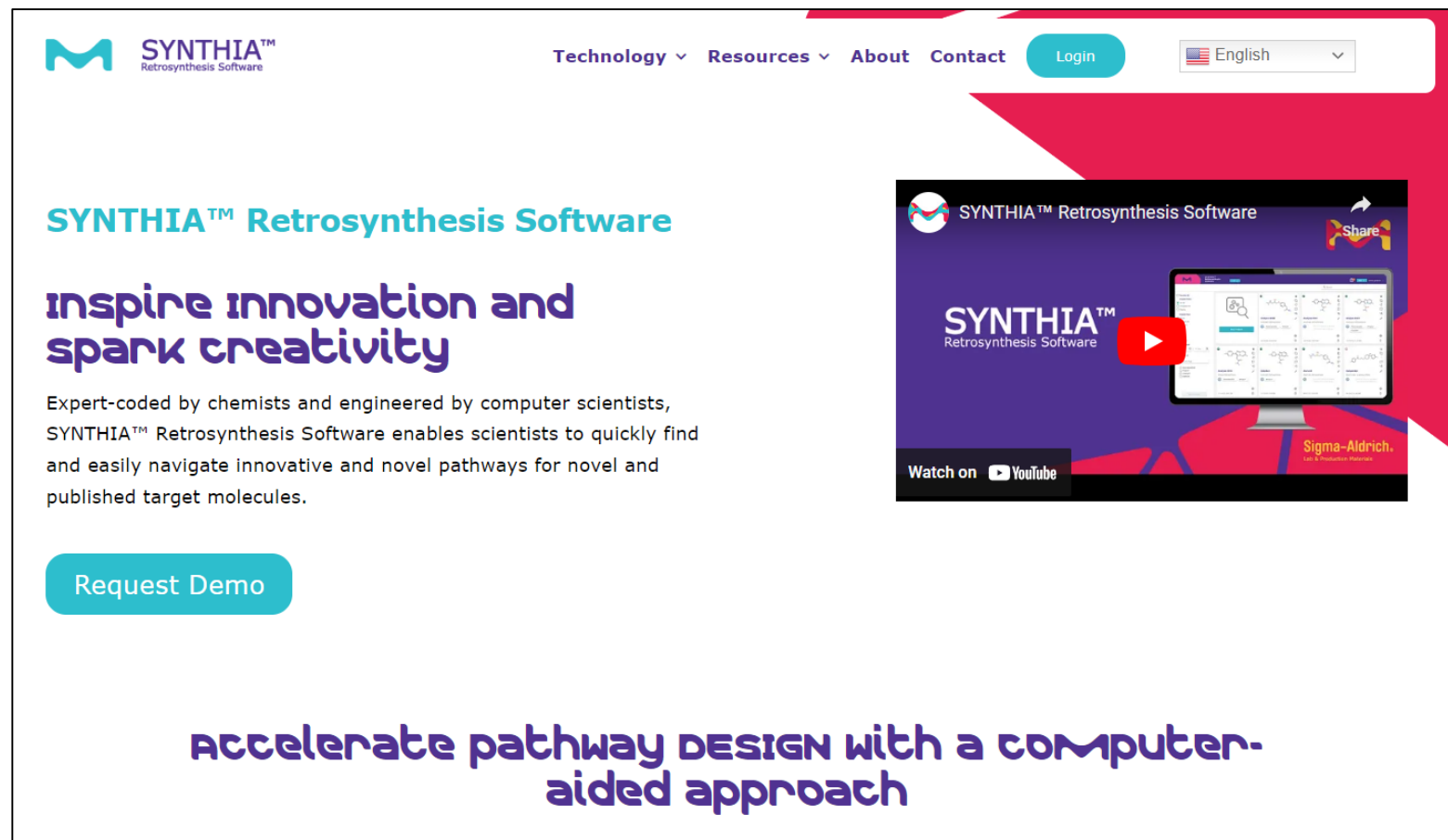
🛒 SEARCH BUYABLES

QM Descriptor

▶ RUN TASK

<https://www.synthiaonline.com/>

<https://www.youtube.com/watch?v=bqJM2HkdMn8&t=173s>



The image shows a landing page for SYNTHIA™ Retrosynthesis Software. The page has a white background with a pink and purple geometric design on the right side. At the top, there is a navigation bar with the SYNTHIA™ logo, a menu with 'Technology', 'Resources', 'About', and 'Contact', a 'Login' button, and a language dropdown set to 'English'. The main heading is 'SYNTHIA™ Retrosynthesis Software' in teal, followed by the tagline 'inspire innovation and spark creativity' in purple. Below this, a paragraph states: 'Expert-coded by chemists and engineered by computer scientists, SYNTHIA™ Retrosynthesis Software enables scientists to quickly find and easily navigate innovative and novel pathways for novel and published target molecules.' A teal 'Request Demo' button is positioned below the text. On the right, there is a video player showing a screenshot of the software interface with a red play button. The video player includes a 'Share' icon, a 'Watch on YouTube' button, and the 'Sigma-Aldrich' logo. At the bottom, a large purple text block reads: 'Accelerate pathway DESIGN with a computer-aided approach'.

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Synthetically Accessible Virtual Inventory (SAVI) Database

[First Full Release](#) | [First Complete Beta Release](#)

SAVI-2020 Full File Series - April 2020

1.75 billion proposed products with reactions generated

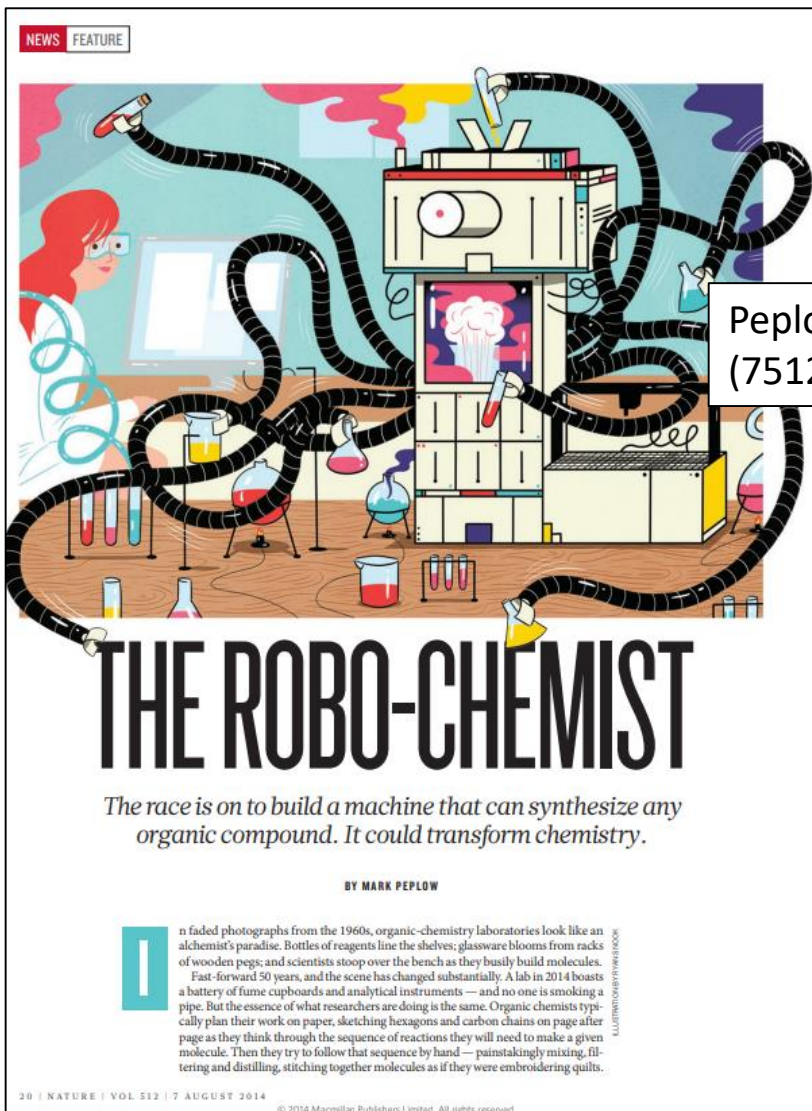
“...this represents only a microscopically small fraction of the drug-like small-molecule space, which has been variously estimated to be on the order of 10^{21} to 10^{63} possible structures or even larger.”

This version utilizes: (a) a set of transforms with rich chemical context annotation including functional group reactivity data and scoring systems (based on the LHASA project, programmed in CHMTRN/PATRAN; see <https://doi.org/10.26434/chemrxiv.11439984.v1>); (b) a set of readily available building blocks in gram quantities (Enamine, Kyiv, Ukraine); (c) the chemoinformatics toolkit CACTVS with custom development (Xemistry GmbH, Glashütten, Germany). For generation of the SAVI-2020 set of products, 53 transforms were used, applied to approx. 150,000 building blocks in single-step reactions. The CHMTRN/PATRAN source code of the transforms can be downloaded [here](#). For a more detailed description of the SAVI project, see <https://doi.org/10.26434/chemrxiv.12185559.v1> and <https://doi.org/10.1038/s41597-020-00727-4>.

Citation: If you want to cite the data themselves, please cite: Patel, H., Ihlenfeldt, W. D., Judson, P. N., Moroz, Y., Pevzner, Y., Peach, M., Tarasova, N., & Nicklaus, M. (2020). Synthetically Accessible Virtual Inventory (SAVI) (Version 2020). CADD Group, CBL, CCR, NCI, NIH, <https://doi.org/10.35115/37N9-5738>. Otherwise, please cite the references above.

License: [Creative Commons Attribution 4.0 International \(CC BY 4.0\)](#).

Patel H, Ihlenfeldt W, Judson P, Moroz YS, Pevzner Y, Peach M, et al. Synthetically Accessible Virtual Inventory (SAVI). ChemRxiv. **2020**;
doi:10.26434/chemrxiv.12185559.v1



Peelow, M. Organic Synthesis: The Robo-Chemist. Nature 2014, 512 (7512), 20–22. <https://doi.org/10.1038/512020a>.

<https://www.nature.com/articles/512020a.pdf>

Unfortunately, those failures are rarely recorded in the literature.

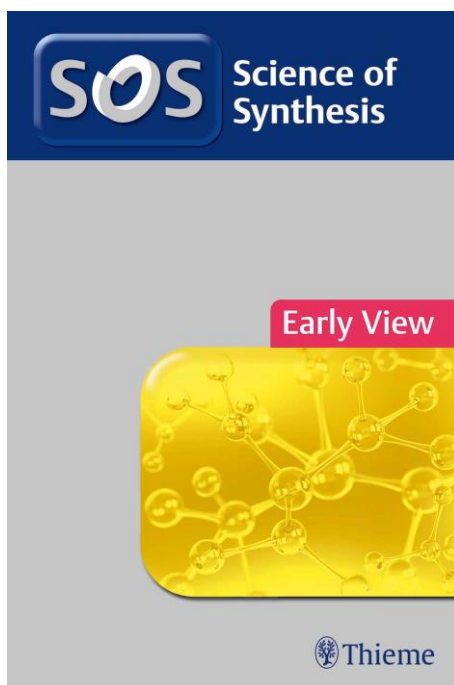
Money is also a significant hurdle.

“A synthesis machine would be transformational... [yet] I can see challenges”



Houben-Weyl Methods of Organic Chemistry

<https://science-of-synthesis.thieme.com/app/search>



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- Electronic Backfile ([less...](#))
 - Science of Synthesis Backfile ([more...](#))
 - Houben-Weyl ([more...](#))

20.2.1.2.11 Synthesis of Carboxylic Acids from Carboxylic Acid Derivatives (Update 2024)

DOI: 10.1055/sos-SD-120-00336



Leclerc, E., *Science of Synthesis Knowledge Updates, early view.*

General Introduction

The synthesis of carboxylic acids from carboxylic acid derivatives has been described previously in *Science of Synthesis* (Section 20.2.1.2), ^[1] and an update to the original contribution on this topic was published in 2011 (Section 20.2.1.2.10). ^[2] The following sections describe either additional methods for known transformations, or the use of new precursors for the preparation of carboxylic acids that were not covered in the original chapter or the first update.

Good Afternoon, Ian

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Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.

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Example: Schubert, J A

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Retrosynthetic Analysis

Make reaction plans with conditions, yields, catalysts, and experimental procedures.



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☐ German (240)

☐ Japanese (220)

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Publication Year



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to

No Max

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☐ 1

New ventures in the construction of complex heterocycles. **Synthesis** of **morphine** and **hasubanan alkaloids**

By: Trauner, Dirk; Porth, Stefanie; Opatz, Till; Bats, Jan W.; Giester, Gerald; Mulzer, Johann

Synthesis (1998), (Spec.), 653-664 | Language: English, Database: CAPlus

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Substances (56)

Reactions (44)

Citing (43)

Citation Map

☐ 2

Formal **synthesis** of (-)-**morphine** from D-glucal based on the cascade Claisen rearrangement

By: Tanimoto, Hiroki; Saito, Ryosuke; Chida, Noritaka

Tetrahedron Letters (2008), 49(2), 358-362 | Language: English, Database: CAPlus

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Full Text

Substances (29)

Reactions (196)

Citing (66)

Citation Map

☐ 3

Enzymatic hydroxylation of arene and symmetry considerations in efficient **synthetic** design of oxygenated natural products

By: Hudlicky, Tomas; Fan, Rulin; Luna, Hector; Olivo, Horacio; Price, John

Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1993), 32B(1), 154-8 | Language: English, Database: CAPlus

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Substances (12)

Reactions (11)

Citing (1)

Citation Map

Morphine synthesis and biosynthesis-an update

1 0 94 Citation Map



In this Reference

- [CAS Concepts](#)
- [Substances](#)
- [Cited Documents](#)

By: Novak, Bennett H.; Hudlicky, Tomas; Reed, Josephine W.; Mulzer, Johann; Trauner, Dirk

DOI: 10.2174/1385272003376292

This review with 106 references covers recent developments in the area of morphine synthesis and biosynthesis. Recent advancements in biosynthesis of morphine alkaloids are discussed. Total syntheses published since 1996 are reviewed and all published approaches to the morphine skeleton are discussed. This review includes an addnl. reference list for synthesis of medicinally important derivatives, improvements in alkaloid interconversion, and a list of all dissertations dealing with morphine synthesis.

Keywords: review morphine alkaloid derivative synthesis biosynthesis

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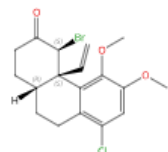
^ Reactions

44

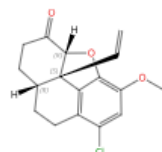
31-614-CAS-25703138

Steps: 1 Yield: 98%

[View Experimental Protocols](#)



Absolute stereochemistry shown,
Rotation (-)

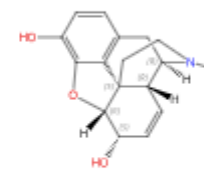


Absolute stereochemistry shown,
Rotation (-)

1.1 Solvents: [Dimethylformamide](#)

^ Substances

57-27-2



Absolute stereochemistry shown, Rotation (-)

$C_{17}H_{19}NO_3$

Morphine

Role: Reactant, Synthetic Preparation, Reactant
or Reagent, Preparation

Notes: derivatives

^ CAS Concepts

Alkaloids

Modifier: morphine-type

Role: Reactant; Synthetic Preparation

Good Afternoon, Ian

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- Molecular Formula

Examples: C₆H₆ | (C₈H₈)_x | C₂₂H₂₆CuN₂O₅.C₂H₃N

+ Add Advanced Search Field



Retrosynthetic Analysis

Make reaction plans with conditions, yields, catalysts, and experimental procedures.



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Draw forms or bonds.

Left Panel (Tools):

- Eraser, Pencil
- Line, Angle, Et, R, X, Fn
- Charge (+, -), Ring closure [1-4], Cyclohexane, Cyclohexene, Cyclohexadiene
- Double bond, Triple bond, A-B, C=C, C≡C
- Arrow, Arrowhead

Right Panel (Elements):

- C, H, O, S, N, P, Cl, Si
- Diagonals, EZ, Rings (5, 6, 7, 8)

Chemical Structure:

Molecular Formula: C₁₇H₁₉NO₃ (285.34)

Taber, D. F.; Neubert, T. D.; Rheingold, A. L. Synthesis of (–)-Morphine. J. Am. Chem. Soc. **2002**, 124 (42), 12416–12417. <https://doi.org/10.1021/ja027882h>.

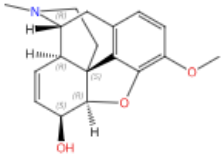
4

Synthesis of (–)-Morphine

By: Taber, Douglass F.; Neubert, Timothy D.; Rheingold, Arnold L.

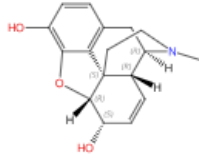
Journal of the American Chemical Society (2002), 124(42), 12416-12417 | Language: English, Database: CAPLUS and MEDLINE

Full Text ▼



Absolute stereochemistry shown, Rotation (–)

Suppliers (29)



Absolute stereochemistry shown, Rotation (–)

Suppliers (27)

31-049-CAS-13524928

Steps: 1 Yield: 86%

1.1
Reagents: [Boron tribromide](#)
Solvents: [Dichloromethane](#)

1.2
Reagents: [Ammonium hydroxide](#)
Solvents: [Water](#)

[Experimental Protocols](#)

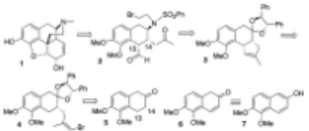
Published on Web 09/28/2002

Synthesis of (–)-Morphine

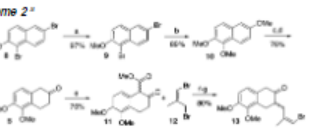
Douglass F. Taber,* Timothy D. Neubert, and Arnold L. Rheingold[†]
Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware 19716
Received July 26, 2002

Morphine (**1**) is the principal alkaloid of opium, derived from *Papaver somniferum* L., or *P. album* Mill., Papaveraceae.¹ Morphine is also found in normal brain, blood, and liver tissue.² The morphine alkaloids comprise a family of structurally related natural products of unique clinical importance in medicine.³ The unusual architecture of morphine has offered a continuing challenge to the art and science of organic synthesis.^{4–6}

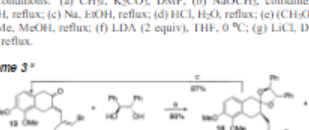
Scheme 1



Scheme 2^a



Scheme 3^a



^a Conditions: (a) CH_3I , K_2CO_3 , DMF; (b) NaOCH_3 , collidine, Cul, MeOH, reflux; (c) Na, EtOH, reflux; (d) HCl, EtO, reflux; (e) $(\text{CH}_3\text{O})_2\text{CO}$, NaOMe, MeOH, reflux; (f) LDA (2 equiv), THF, 0 °C; (g) LiCl, DMSO, H₂O, reflux.

Our approach to the synthesis of (–)-morphine **1** began with the preparation of β -tetralone **13** (Scheme 2). Using modifications of the published procedures,⁸ we alkylated 1,4-dibromo-2-naphthol **8** with iodomethane to give the methoxynaphthalene **9**. Ullman coupling with sodium methoxide then gave the desired trimethoxynaphthalene **10**. Dissolving metal reduction followed by hydrolysis led to the desired β -tetralone **5**. The β -tetralone **5** would tend to alkylate at the benzylic position. The procedure of Aristoff,⁹ methoxycarbonylation, dianion alkylation using *cis*-1,3-dibromo-2-methyl-1-propene,¹⁰ and decarboxylation, was therefore employed to obtain the alkylated β -tetralone **13**.

Protection of the β -tetralone **13** (Scheme 3) with (5*S*)-(–)-hydrobenzoin gave the diastereomeric ketals **14** and **4**, which, as anticipated, were separable by silica gel chromatography. The undesired diastereomer **14** was readily recycled to the racemic β -tetralone **13**. Cyclization of ketal **4** via alkylidene carbene C–H insertion¹¹ followed by hydrolysis led to the enantiomerically pure ketone **15**. The beauty of this approach is that while β -tetralone **13** can readily racemize, β -tetralone **15** cannot.

The sterically congested ketone **15** was selectively reduced to the *cis* alcohol **16**. Direct displacement of the alcohol by a functionalized amine could not be achieved. Fortunately, the alcohol

16 was smoothly converted to the azide via Mitsunobu coupling. Reduction and protection then gave sulfonamide **17**.

The key to the assembly of morphine was the anticipated selective bis-cyclization of keto aldehyde **2** (Scheme 4). Alkylation of the sulfonamide **17** with 1,2-dibromoethane under phase-transfer conditions provided **18**, which upon ozonolysis gave the desired keto aldehyde **2**. The benzylic proton α to the aldehyde in **2** is the most acidic, so we expected to obtain the aldehyde enolate selectively. Although the keto aldehyde **19** could be isolated after brief exposure to base, it was more practical to continue heating, to cleanly obtain the tetracycle **20**. The final conversion to complete the core structure of morphine **1** was the construction of the ether ring. Reduction of the enone **20** gave a single alcohol **21** (Scheme

[†] To whom correspondence should be addressed. E-mail: taberdf@udel.edu.
[‡] For X-ray analysis.

12416 • J. AM. CHEM. SOC. 2002, 124, 12416–12417

10.1021/ja027882h CCC: \$22.00 © 2002 American Chemical Society

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Reactions for 57-27-2

References



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Substance Role

☒ Product (122)

Yield

☐ No Yield Available (122)

Number of Steps

☐ 1 (40)

☒ 2 (25)

☒ 3 (27)

☒ 4 (33)

☒ 5 (37)

☐ 6-10 (331)

☐ 11-15 (563)

☐ 16-20 (129)

☐ >20 (6)

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Substance Role: Product X

Number of Steps: 4 Selected X

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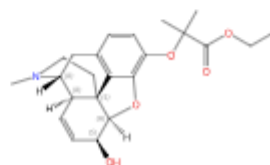
Group: By Scheme

Sort: Yield

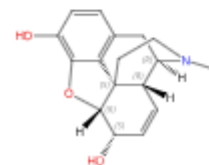
View: Expanded

Scheme 1 (1 Reaction)

Steps: 2



Absolute stereochemistry shown



Absolute stereochemistry shown, Rotation (-)

Suppliers (27)

☐ [View Reaction Detail](#)

Steps: 2

[Synthesis of metabolites of 3-O-tert-butylmorphine](#)

1.1 Reagents: [Lithium aluminum hydride](#)

Solvents: [Tetrahydrofuran](#)

2.1 Reagents: [Pyridinium chloride](#)

By: Mohacsi, E.

Journal of Heterocyclic Chemistry (1987), 24(2), 471-2

[Full Text](#)

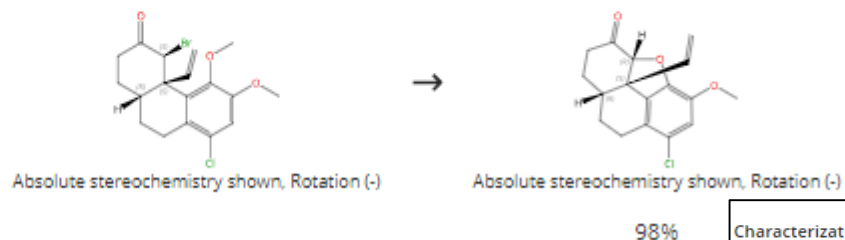
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Scheme 2 (2 Reactions)

Steps: 2

CAS Reaction Number: 31-614-CAS-25703138

Get Similar Reactions



Characterization Data

Phenanthro[4,5-*bcd*]furan-3(2*H*)-one, 7-chloro-9*b*-ethenyl-1,3*a*,8,9,9*a*,9*b*-hexahydro-5-methoxy-, (3*aR*,9*aR*,9*bS*)-

Proton NMR Spectrum 250 MHz, CDCl₃: δ (dq, 1 H, *J* = 4.9, 12.6 Hz), 1.70-2.20 (m, 3 H), 2.23-2.45 (m, 4 H), 2.61 (ddd, 1 H, *J* = 0.9, 7.3, 18.0 Hz), 3.82 (s, 3 H), 4.52 (dd, 1 H, *J* = 0.7, 17.0 Hz), 4.71 (s, 1 H), 5.14 (dd, 1 H, *J* = 0.7, 10.2 Hz), 5.97 (dd, 1 H, *J* = 10.2, 17.0 Hz), 6.71 (s, 1 H).

Carbon-13 NMR 63 MHz, CDCl₃: δ 22.9, 26.5, 36.1, 39.4, 55.2, 56.6, 91.7, 114.7, 117.1, 123.9, 125.0, 126.8, 141.8, 142.9, 145.6, 206.5.

IR Absorption Spectrum Si: ν = 2938, 1729, 1631, 1491, 1436, 1186, 1147, 1096, 1037, 973, 873 cm⁻¹.

Optical Rotatory Power [α]_D -35.7, (c = 2, CHCl₃).

Elemental Analysis C₁₇H₁₇ClO₃ (304.8): calcd C, 67.00; H, 5.62; found C, 66.92; H, 5.55.

HRMS *m/z* calcd for C₁₇H₁₇ClO₃ 304.08662, found: 304.08662 ± 0.0015.

Mass Spectrum EI, 70 eV, 30°C: *m/z*(%) = 306 (57), 304 (M⁺, 99), 244 (87), 174 (76), 149 (28), 131 (41), 95 (33), 69 (100).

Melting Point 147-148 °C (racemic), 178-179 °C (enantio-merically pure).

R_f 0.25 (hexane/EtOAc, 3:1).

State colorless crystals.

Experimental Protocols

Synthetic Methods

Experimental Procedure

Products [Phenanthro\[4,5-*bcd*\]furan-3\(2*H*\)-one, 7-chloro-9*b*-ethenyl-1,3*a*,8,9,9*a*,9*b*-hexahydro-5-methoxy-, \(3*aR*,9*aR*,9*bS*\)-](#), Yield: 98%

Reactants [\(4*S*,4*aS*,10*aR*\)-4-Bromo-8-chloro-4*a*-ethenyl-1,4,4*a*,9,10,10*a*-hexahydro-5,6-dimethoxy-3\(2*H*\)-phenanthrenone](#)

Solvents [Dimethylformamide](#)

Procedure

1. Heat a solution of bromoketone derivative (3.99 g) in anhydrous DMF (50 mL) to 140 °C for 20 minutes.
2. Cool the solution to room temperature.
3. Remove the solvent in vacuo.
4. Purify the crystalline crude product by chromatography on silica gel, eluting with hexane/EtOAc (1/1).

Scale gram

Retrosynthesis Plan for drawn structure

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Key Experimental Steps Predicted Steps [Edit Plan Options](#)

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Plan Information

Estimated Yield: 28%
Overall Price: \$251,818.60
(USD per 100 grams)

Scoring Profiles

Complexity Reduction

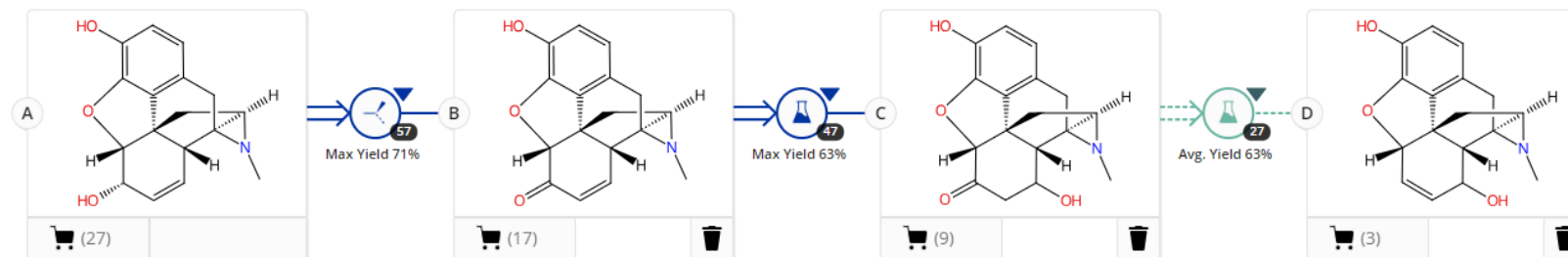
Convergence

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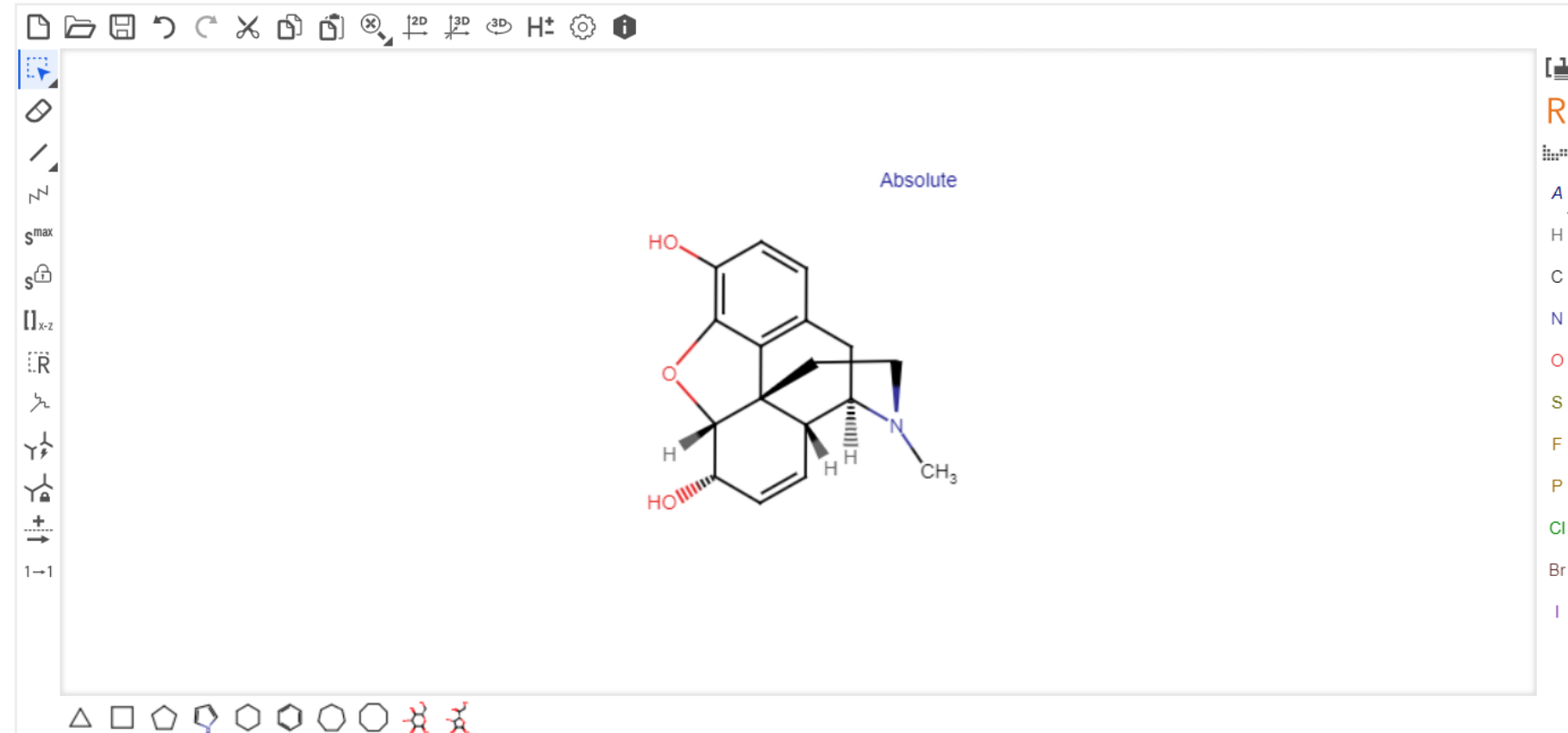
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1

CC(=O)OC(=O)C + CN1[C@H]2[C@H]3[C@H]([C@@H]1O)C[C@H]([C@@H]2O)C4=CC=C(C=C4)O → CC(=O)OC1=CC=C2[C@H]3[C@H]([C@@H]1O)C[C@H]([C@@H]2O)C4=CC=C(C=C4)N3

28

7

1

9 Conditions Find Similar Reaction ID: 832970

Conditions	Yield	Reference
With sodium hydrogencarbonate In water at 20°C; for 0.25h; Experimental Procedure 	99%	Ahonen, Tiina J.; Rinne, Maiju; Grutschreiber, Peter; Mätlik, Kert; Airavaara, Mikko; Schaarschmidt, Dieter; Lang, Heinrich; (...) Yli-Kauhaluoma, Jari; Moreira, Vânia M. [European Journal of Medicinal Chemistry, 2018, vol. 151, p. 495 - 507] Full Text  Cited 3 times  Details  Abstract 
With phosphate buffer pH=7; Acetylation;	90%	Berrang, Bertold D.; Wyrick, Christopher D.; Carroll, F. Ivy; Seltzman, Herbert H. [Journal of labelled compounds and radiopharmaceuticals, 1999, vol. 42, # 9, p. 851 - 857] Full Text  Cited 5 times  Details  Abstract 



1



1 Conditions [Find Similar](#) > Reaction ID: 20800136

Conditions

Yield

Reference

Multi-step reaction with 11 steps

- 1: 77 percent / H₂ / 5 percent Pd/C / ethyl acetate / 735.5 Torr
- 2: 1.) pyridine / 1.) 0 deg C, 1 h; 2.) water, 30 min
- 3: 39 g / imidazole / dimethylformamide; CH₂Cl₂ / 1.) RT, 2 h; 2.) 45 deg C, 20 h; 3.) 80 deg C, 3 h
- 4: 82.6 percent / 85 percent KOH / methanol; benzene / 2.5 h / Ambient temperature
- 5: 96 percent / pyridinium chlorochromate / CH₂Cl₂ / 1 h
- 6: 63 percent / tetrahydrofuran; CH₂Cl₂ / 1.5 h / -78 °C
- 7: 99 percent / 4-N,N-dimethylaminopyridine / pyridine / 1.5 h
- 8: 1.) ozone; 2.) dimethylsulfide / 1.) MeOH, -78 deg C, 10 min; 2.) -10 deg C, 1 h, 0 deg C 1 h, RT, 1 h
- 9: 95 percent / Et₃N / CH₂Cl₂ / 40 h / Ambient temperature
- 10: 81 percent / 42 h / 50 °C
- 11: 82 percent / 4.4M NaOMe / methanol; tetrahydrofuran / 28.5 h

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[Wovkulich; Barcelos; Batcho; et al.](#)

[**Tetrahedron**, **1984**, vol. 40, # 12, p. 2283 - 2296]

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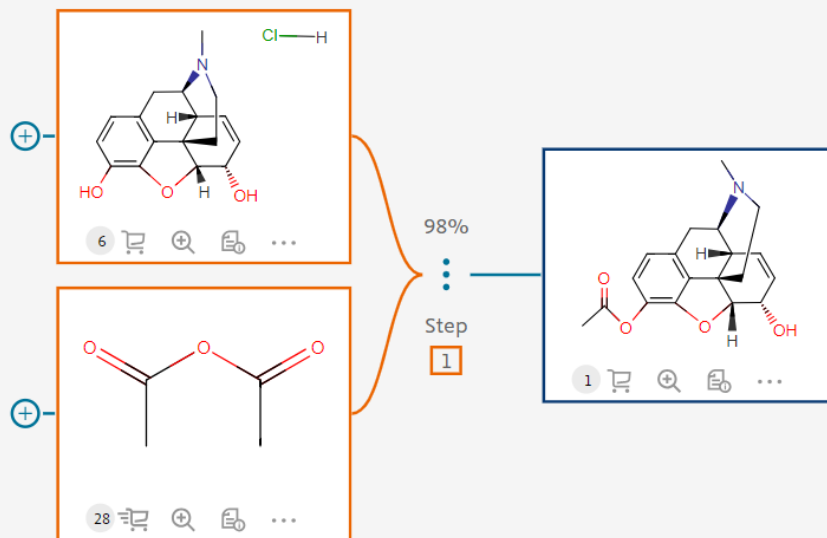
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Step 1

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	Conditions	Yield	Reference
☐	With sodium hydrogencarbonate In water at 20°C; Experimental Procedure	98%	Váradi, András; Hosztafi, Sándor; Le Rouzic, Valerie; Tóth, Gergo; Urai, Ákos; Noszál, Béla; Pasternak, Gavril W.; Grinnell, Steven G.; Majumdar, Susruta [European Journal of Medicinal Chemistry, 2013, vol. 69, p. 786 - 789] Full Text Cited 15 times Details
☐	Stage #1: morphine hydrochloride With sodium hydrogencarbonate In water at 20°C; Stage #2: acetic anhydride In water at 20°C; for 1h;		Váradi, András; Gergely, András; Béni, Szabolcs; Jankovics, Péter; Noszál, Béla; Hosztafi, Sándor [European Journal of Pharmaceutical Sciences, 2011, vol. 42, # 1-2, p. 65 - 72] Full Text Cited 17 times Details



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Nielsen, S; Degenhardt, L; (...); Gisev, N



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PurposeOral Morphine Equivalent (OME) doses are increasingly being used as a metric to represent opioid use. Driven by a growing need from pharmacoepidemiological studies, the objective of this study was to develop a comprehensive OME conversion table that can be used by researchers to calculate OMEs in a consistent and systematic way ... [Show more](#)

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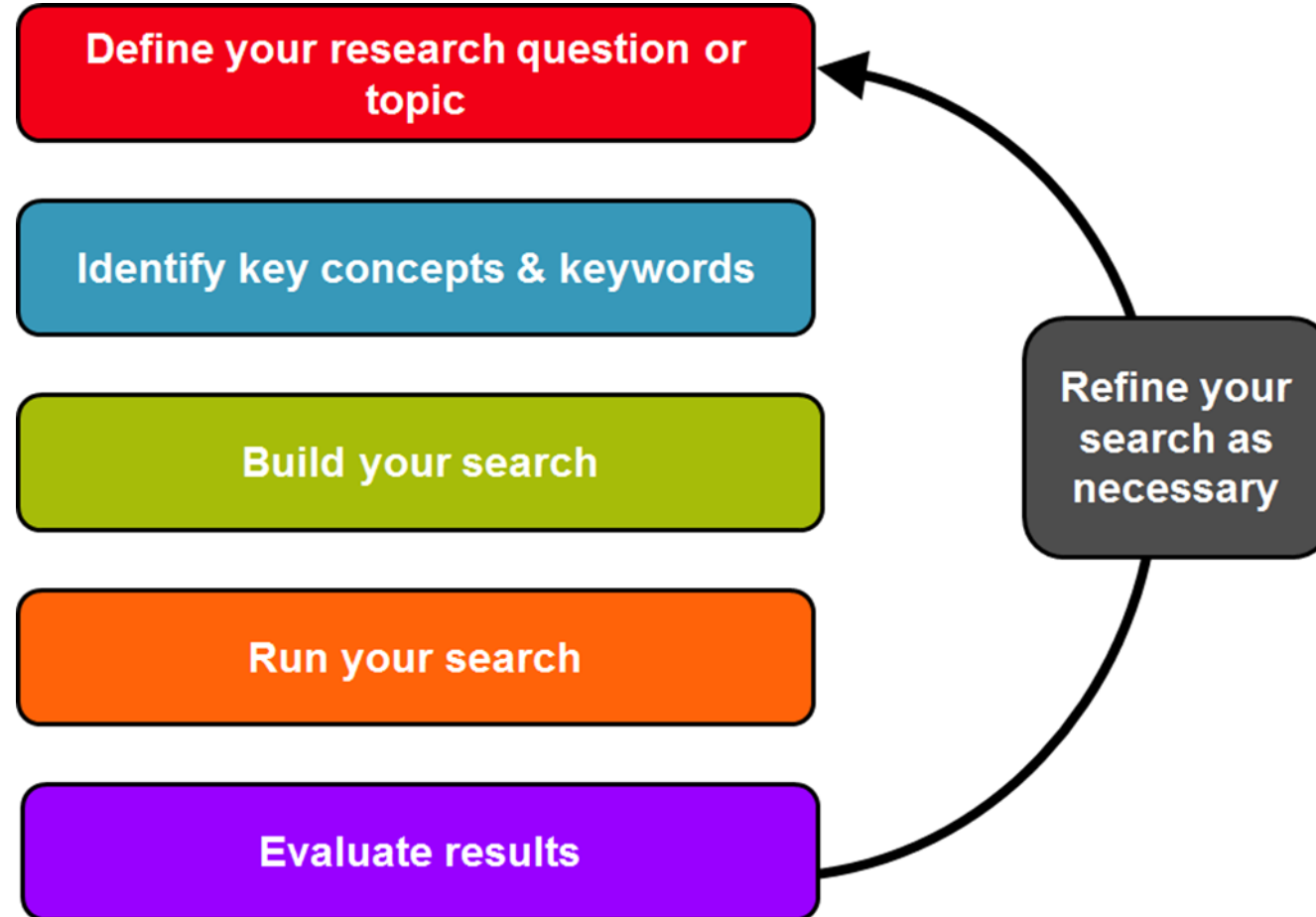
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Allen, RS; Millgate, AG; (...); Larkin, PJ

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- CHEM Library Research Guide
- Databases – lots of them!
- Citation management
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(1) Novak, B.; Hudlicky, T.; Reed, J.; Mulzer, J.; Trauner, D. Morphine Synthesis and Biosynthesis-An Update. *COC* **2000**, 4 (3), 343-362.
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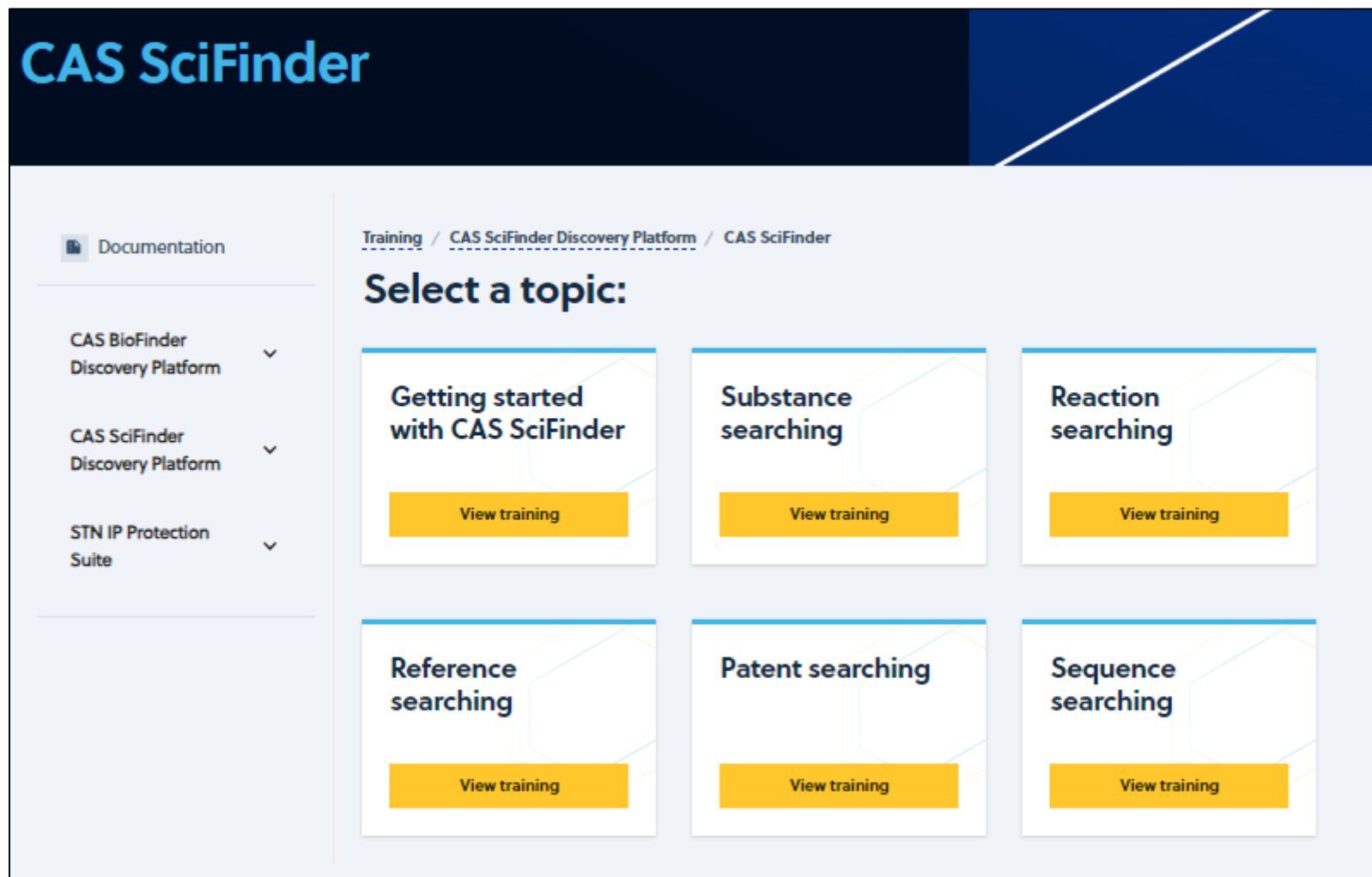
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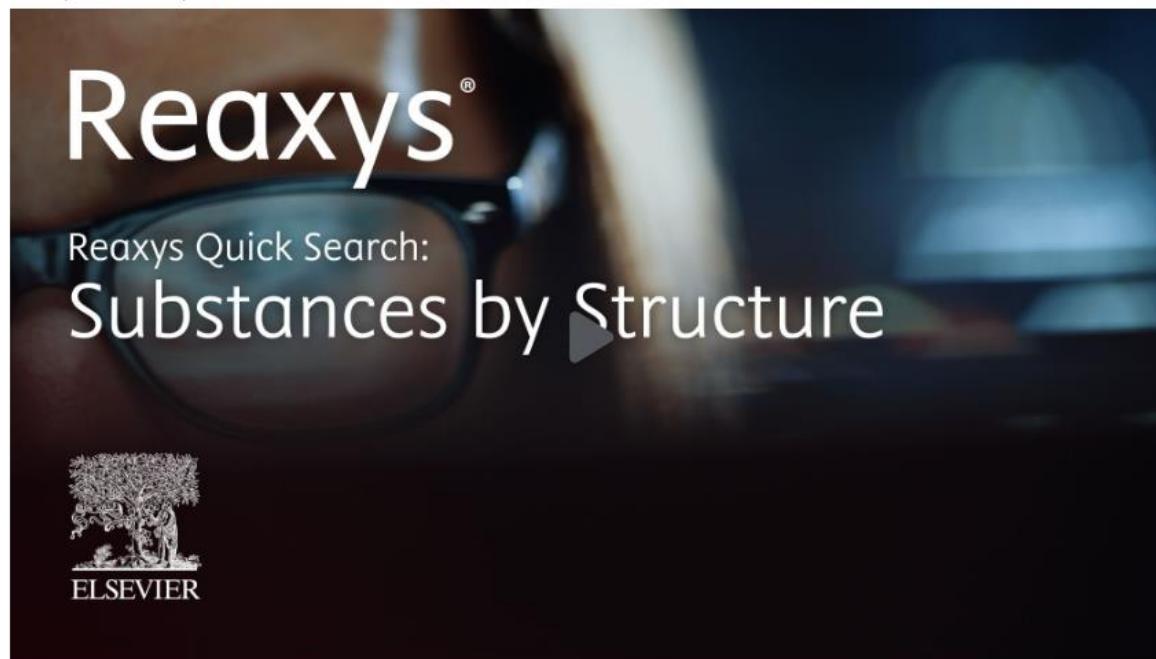
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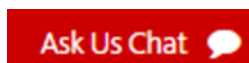
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